

Multiscale Characterization of bcc Crystals Deformed to Large Extents of Strain



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Experimental data are crucial in the process of construction and validation of multiscale crystal plasticity models, used in computer code simulations of materials deformed under extreme conditions such as high strain rate, pressure, and large extents of strain. The “6 Degrees of Freedom” experiment was designed specifically for validation of plasticity simulations and has provided data on the behavior of body-centered cubic (bcc) crystals that may well revolutionize how crystal plasticity models are developed and implemented in computer code simulations.

The experimental data and simulation efforts, however, have focused on relatively small extents of plastic deformation (0.5%). Both experiments and modeling must now be extended to large-strain deformations on the order of tens of percent. At these larger extents of strain, multiscale characterization tools can be better used to understand the fundamental behavior.

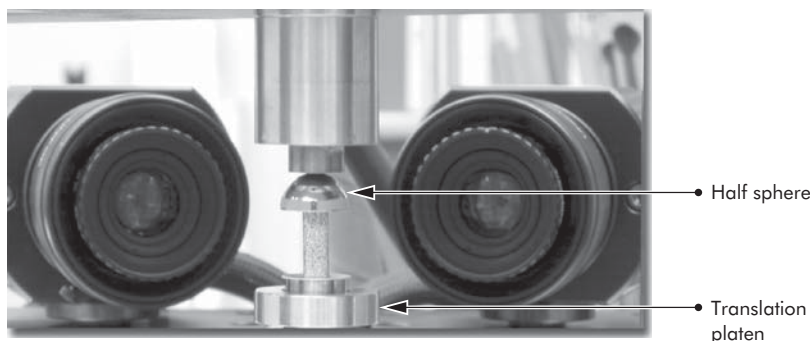


Figure 1. Photograph of the large-strain testing set-up.

Project Goals

Our goal is to develop large-strain experiments that will provide the essential data to enhance the multiscale modeling capability, through the creation of continuum strength models and the validation of future simulations. When completed, this work will increase the Laboratory’s ability to develop predictive strength models for use in computer code simulations.

Relevance to LLNL Mission

Understanding and simulating the plastic, or nonreversible, deformation of bcc metals, is a major component of LLNL’s Stockpile Stewardship Program and is intended to simulate future NIF experiments.

FY2004 Accomplishments and Results

Our accomplishments and results include:

Strain and slip system measurement. A commercial 3-D image correlation system was purchased and is being used in our deformation experiments to measure the strain nonuniformities in the sample. A picture of the set-up is shown in Fig. 1. Figure 2 shows a strain map of the image correlation result from a compression experiment performed on a single crystal Mo sample. Figure 2 also shows the corresponding stress and strain data in comparison with strain gage data. The close match between the two experiments verifies the accuracy of the image correlation technique. We have also performed a detailed analysis of the slip traces on the surface of the sample, and using that

information, have calculated the slip system activity that is consistent with the experimental data.

Stress State. A detailed FEM analysis has been performed on a deformed sample to examine the nonuniformities in the stress state. The analysis shows that at 2% strain the uniaxial stress in the sample varies by $\pm 20\%$.

Large strain validation experiment. The development of a massively parallel dislocation dynamics code (ParaDis) has led to the ability to perform a dislocation-dynamics (DD) simulation to 3% strain. An experiment on a symmetrically oriented sample tested at 500 K to 10% strain has been conducted for the purpose of validating the simulation. The results of the experiment in comparison to the DD simulation show that while qualitatively the results appear similar, quantitatively, there

is nearly a 4- \times difference in the stress values. Although there is still large disparity between the simulation and the experiments, this comparison is the first step in increasing interactions between experimentalists and modelers to understand the necessary physical parameters required for future validation tests.

Related References

1. Bulatov, V. V., "Current Developments and Trends in Dislocation Dynamics," *J. Computer-Aided Mat. Design*, **9**, p. 133, 2002.
2. Lassila, D. H., M. M. Leblanc, and G. J. Kay, "Uniaxial Stress Deformation Experiments for Validation of 3-D Dislocation Dynamics Simulations," *J. Eng. Mat. Tech.*, **124**, p. 290, 2002.
3. Schmidt, T., J. Tyson, and K. Galanulis, "Full-Field Displacement and Strain Measurement Using Advanced 3D Image Correlation," *Photogrammetry: Part I, Exp. Techniques*, **27**, p. 47, 2003.

FY2005 Proposed Work

A second pair of cameras has been purchased and will be incorporated into our existing experimental set-up. We will continue to remachine and test single crystal Mo samples to achieve larger strains. Characterization of the deformed samples in collaboration with the University of California, Berkeley, will also continue. We will also begin performing experiments on Ta single crystals. The results of these experiments and characterizations will be compared with simulations to further the understanding of the deformation mechanisms in these materials and to begin validation of the DD code.

Accurate validation experiments out to large extents of strain are still required for the continued development of computer code simulation capabilities.

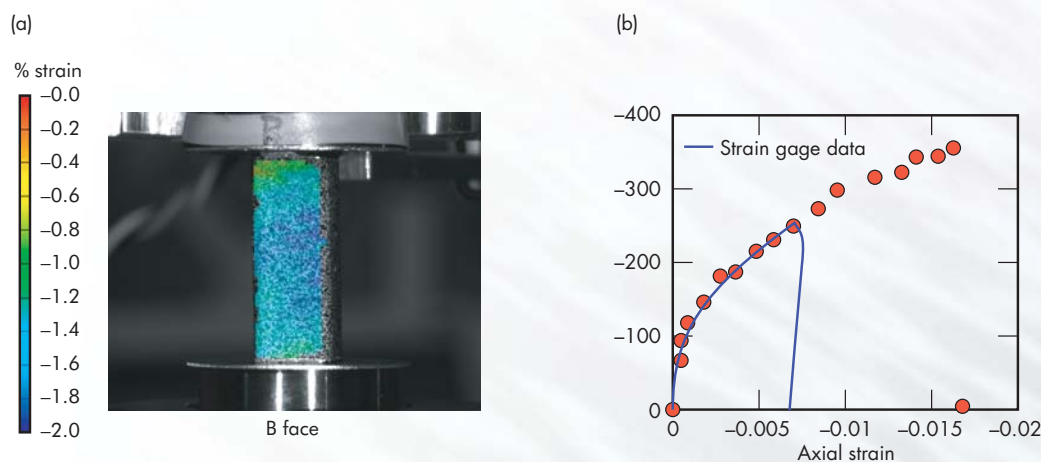


Figure 2. (a) Axial strain results using the image correlation system. (b) Corresponding stress/strain curve. The axial strains are calculated by averaging over an area similar to the active region of a strain gage.